A2

--4. A method which comprises:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type of covalent bonds and three-dimensional coordinates for each atom of a ligand;

covering all possible docking structures between said biopolymer and said ligand while changing the conformation of said ligand by rotating torsion angles for each binding scheme; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable docking structure relative to the biopolymer, the stability of said docking structures, as well as the binding modes and conformations of the ligand in said structures,

wherein only stable docking structures are output by using structure-optimization steps of torsion angles in the ligand together with relative positions and orientations between the biopolymer and ligand.

5. A method which comprises:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type of covalent bonds and three-dimensional coordinates for each atom of a ligand;

selecting stable docking structures between said biopolymer and said ligand based on calculated energies while changing the conformation of said ligand by rotating torsion angles for each hydrogen-bonding scheme; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable docking structure